Error Estimation for the Clenshaw-Curtis Quadrature Method

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Error Estimation for the Clenshaw-Curtis Quadrature Method

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Dedicated to the Memory of Professor Dr. Stefan Schottlaender

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1. Introduction

The numerical computation of a given functional I of the type

$$I[f] := \int_{-1}^{1} f(x)k(x)\,dx\,, \quad k \in L^1 \tag{1}$$

is mostly done by functionals Q ("quadrature rules") of the type

$$Q[f] := \sum_{\nu=1}^{n} a_\nu f(x_\nu)\,, \quad x_\nu \in [-1,1]\,.$$

The error is the functional $R := I - Q$. The degree of Q is the number $\deg[Q] := \sup\{m \mid R[\mathcal{P}_m] = 0\}$, where $\mathcal{P}_m$ denotes the space of polynomials of degree at most m.

Starting point of many investigations of the error is the PEANO kernel theorem (e. g. BRASS [2]): If $\deg[Q] \geq s-1$ holds, then we have

$$R[f] = \int_{-1}^{1} f^{(s)}(x)K_s(x)\,dx \tag{2}$$

with

$$K_s(x) := R\left[\frac{(\cdot - x)_+^{s-1}}{(s-1)!}\right]\,. \tag{3}$$

K_s is called the s-th PEANO kernel of the rule Q.

An immediate consequence of (2) is the best possible error bound

$$\left|R[f]\right| \leq \varrho_s(Q) \sup_{-1\leq x\leq 1} \left|f^{(s)}(x)\right| \tag{4}$$

with

$$\varrho_s(Q) := \int_{-1}^{1} \left|K_s(x)\right|\,dx\,. \tag{5}$$

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A further (not quite immediate) consequence of (2) is the best possible error bound

$$\left|R[f]\right| \leq \phi_s(Q)\,\mathrm{Var}\left[f^{(s-1)}\right] \tag{6}$$

with

$$\phi_s(Q) := \sup_{-1\leq x\leq 1}\left|K_s(x)\right|, \tag{7}$$

where Var denotes the total variation.

Using a computer, we can evaluate $\varrho_s(Q)$ and $\phi_s(Q)$ for a given quadrature rule Q without any difficulty. We have a deeper problem, if a sequence Q_1, Q_2, ... of quadrature rules with increasing number of evaluation points (a "quadrature method") is given and we want to determine the asymptotic behaviour of $\varrho_s(Q_n)$ and $\phi_s(Q_n)$. The main difficulty is the complicated structure of K_s. It is the aim of this paper to overcome this difficulty in the special case of the CLENSHAW-CURTIS quadrature method by giving a nice and workable approximation of K_s.

The n-th CLENSHAW-CURTIS quadrature rule Q_n^{CC} is defined by its evaluation points

$$x_\nu = x_{\nu,n}^{\mathrm{CC}} := -\cos\frac{\nu-1}{n-1}\pi\,, \qquad \nu = 1,2,\ldots,n\,,$$

together with the condition $\deg\left[Q_n^{\mathrm{CC}}\right] \geq n-1$.

An important theorem of SLOAN and SMITH [4] asserts that

$$\lim_{n\to\infty} Q_n^{\mathrm{CC}}[f] = \int_{-1}^{1} f(x)k(x)\,dx$$

holds for all continuous functions f, if $k \in L^p$ for some $p > 1$. The generality of this theorem with respect to the weight function k makes the CLENSHAW-CURTIS method at present one of the most interesting quadrature methods.

2. The result

We recall the definition of the BERNOULLI functions B_s

$$B_s(x) := -2\sum_{\nu=1}^{\infty}\frac{\cos\left(2\nu\pi x - \frac{s}{2}\pi\right)}{(2\nu\pi)^s}\,. \tag{8}$$

It is well known that the restriction of B_s to $]0,1[$ is a polynomial of degree s.

We can now formulate the basic theorem of this paper

Theorem Let k be a function defined on $[-1,1]$ such that $\hat{k}(x) := k(x)\sqrt{1-x^2}$ is continuous and of bounded variation. Let Q_{n+1}^{CC} be the CLENSHAW-CURTIS quadrature rule with $n+1$ evaluation points for the functional (1). Denote by K_s the s-th PEANO kernel of Q_{n+1}^{CC}. Then we have

$$K_s(x) = \left(\frac{\pi}{n}\right)^s B_s\left(\frac{n\arccos x}{\pi}\right)k(x)\left(1-x^2\right)^{\frac{s}{2}} + o(n^{-s})\,. \tag{9}$$

The o-term holds uniformly in x. If $k=1$, $o(n^{-s})$ may be replaced by $O(n^{-s-1})$.

The proof is given in section 3.

Corollary 1 Under the assumptions of the theorem we have

$$\varrho_s\left(Q_{n+1}^{CC}\right) = \left(\frac{\pi}{n}\right)^s \int_0^1 \left|B_s(u)\right| du \int_{-1}^1 \left|k(x)\right| \left(1-x^2\right)^{\frac{s}{2}} dx \; + \; o(n^{-s}).$$

If $k=1$, then $o(n^{-s})$ may be replaced by $O(n^{-s-1})$.

Proof of the Corollary: From (5) and the theorem we have

$$\begin{aligned}
\varrho_s\left(Q_{n+1}^{CC}\right) &= \left(\frac{\pi}{n}\right)^s \int_{-1}^1 \left|B_s\left(\frac{n \arccos x}{\pi}\right) k(x)\right| \left(1-x^2\right)^{\frac{s}{2}} dx \; + \; o(n^{-s}) \\
&= \left(\frac{\pi}{n}\right)^s \pi \int_0^1 \left|B_s(nt)\, k\left(\cos \pi t\right)\right| \left(\sin \pi t\right)^{s+1} dt \; + \; o(n^{-s}) \\
&= \left(\frac{\pi}{n}\right)^s \int_0^1 \left|B_s(u)\right| du \, \pi \int_0^1 \left|k(\cos \pi t)\right| (\sin \pi t)^{s+1} dt \\
&\quad + \left(\frac{\pi}{n}\right)^s \pi \int_0^1 \left(\left|B_s(nt)\right| - \int_0^1 \left|B_s(u)\right| du\right) \left|k(\cos \pi t)\right| (\sin \pi t)^{s+1} dt \; + \; o(n^{-s}).
\end{aligned}$$

If we now apply the following lemma to the last term, then we obtain the desired result immediately.

Lemma 1 Let h be a bounded integrable function with period 1 and mean value zero (on $[0,1]$). If g is of bounded variation, then

$$\int_0^1 g(t) h(nt)\, dt = O(n^{-1}).$$

Proof: It is sufficient to prove the assertion with the added hypothesis of monotonicity of g. Then we can apply the second mean value theorem:

$$\begin{aligned}
\left|\int_0^1 g(t) h(nt)\, dt\right| &= \left|g(0) \int_0^\xi h(nt)\, dt \; + g(1) \int_\xi^1 h(nt)\, dt\right| = \left|\left(g(0)-g(1)\right) \int_0^\xi h(nt)\, dt\right| \\
&= \left|\frac{g(0)-g(1)}{n} \int_0^{n\xi} h(u)\, du\right| = \left|\frac{g(0)-g(1)}{n} \int_{\lfloor n\xi \rfloor}^{n\xi} h(u)\, du\right| \\
&\le \frac{|g(0)-g(1)|}{n} \sup_u \left|h(u)\right|.
\end{aligned}$$

Corollary 2 Under the assumptions of the theorem we have

$$\phi_s\left(Q_{n+1}^{CC}\right) = \left(\frac{\pi}{n}\right)^s \sup_x \left|B_s(x)\right| \sup_x \left(|k(x)| \, (1-x^2)^{\frac{s}{2}}\right) \; + \; o(n^{-s}).$$

Taking into consideration the continuity of $k(x)\,(1-x^2)^{\frac{s}{2}}$ and the periodicity of B_s, we get this corollary immediately from (7) and (8).

In an important paper PETRAS [3] has given approximations for PEANO kernels of rather general quadrature methods. But he needs some boundedness assumptions which could be proved only for positive quadrature rules. In the class considered here the positivity is known only for the special weight functions $k(x)=1$ and $k(x)=(1-x^2)^{-\frac{1}{2}}$. For these weight functions Corollary 1 (but not Corollary 2) is contained in the results of PETRAS, and (9) can — at least for $x \in [a,b] \subset]-1,1[$ — be derived from expressions given by PETRAS.

3. Proof of the theorem

The central idea of the proof is the expansion of the PEANO kernel in terms of CHEBYSHEV polynomials T_n ($T_n(x) := \cos(n \arccos x)$). According to (3) we should begin with the expansion

$$\frac{1}{s!}(t-x)_+^s = \sum_{\nu=0}^{\infty} a_\nu^{(s)} T_\nu(t)\,, \qquad s=0,1,\ldots, \qquad a_\nu^{(s)} = a_\nu^{(s)}(x). \tag{10}$$

Introducing new variables by $x=\cos\xi$ and $t=\cos\tau$, we get from (10)

$$\frac{1}{s!}\Big(\cos\tau - \cos\xi\Big)_+^s = \sum_{\nu=0}^{\infty} a_\nu^{(s)} \cos\nu\tau\,. \tag{11}$$

The existence and convergence (uniform convergence if $s \geq 1$) of this expansion can be deduced from the elements of FOURIER series theory, we have now to determine the $a_\nu^{(s)}$.

We assume $\tau \in [0,\pi]$ and $\xi \in [0,\pi]$.

<u>Lemma 2</u> If $\nu > s$, then

$$a_\nu^{(s)} = \frac{1}{\pi 2^{s-1}} \sum_{\kappa=0}^{s} (-1)^\kappa \binom{s}{\kappa} \frac{\sin\Big((\nu-s+2\kappa)\xi\Big)}{(\nu-s+\kappa)(\nu-s+\kappa+1)\cdots(\nu+\kappa)}\,.$$

Proof: We use induction on s. We begin with

$$\Big(\cos\tau - \cos\xi\Big)_+^0 = a_0^{(0)} + \frac{2}{\pi}\sum_{\nu=1}^{\infty} \frac{\sin\nu\xi}{\nu}\cos\nu\tau\,.$$

This is a well known result of the theory of FOURIER series. The induction step is done by multiplication with $\frac{1}{s+1}\Big(\cos\tau-\cos\xi\Big)$, I omit the elementary computation.

<u>Lemma 3</u>

$$a_\nu^{(s)} = \frac{2}{\pi}\nu^{-s-1}(\sin\xi)^s \sin\Big(\nu\xi - s\frac{\pi}{2}\Big) \;+\; O(\nu^{-s-2})\,.$$

The O-term holds uniformly in ξ.

Proof: The assertion follows from Lemma 2 by using

$$\frac{1}{(\nu-s+\kappa)(\nu-s+\kappa+1)\cdots(\nu+\kappa)}=\nu^{-s-1}+O(\nu^{-s-2})$$

and

$$\sum_{\kappa=0}^{s}(-1)^{\kappa}\binom{s}{\kappa}\sin\Big((\nu-s+2\kappa)\xi\Big)=(2\sin\xi)^{s}\sin\Big(\nu\xi-s\frac{\pi}{2}\Big)\,.$$

The first relation is trivial, the second can be proved in the usual manner by application of $\sin u=\operatorname{Im}(e^{iu})$ and the binomial theorem.

<u>Lemma 4</u> If λ and n are natural numbers and if $l\in\{0,1,\ldots,n\}$, then

$$Q_{n+1}^{\mathrm{CC}}\Big[T_{2\lambda n\pm l}\Big]=I[T_l]\,.$$

Proof: Because of $T_l\in\mathcal{P}_n$ we have $I[T_l]=Q_{n+1}^{\mathrm{CC}}[T_l]$. The equation $Q_{n+1}^{\mathrm{CC}}\Big[T_{2\lambda n\pm l}\Big]=Q_{n+1}^{\mathrm{CC}}[T_l]$ is an easy consequence of $T_{2\lambda n\pm l}\Big(x_{\nu,n+1}^{\mathrm{CC}}\Big)=T_l\Big(x_{\nu,n+1}^{\mathrm{CC}}\Big)$. But this identity follows immediately from the definitions of T_n and $x_{\nu,n+1}^{\mathrm{CC}}$.

In the following text we shall write a_ν instead of $a_\nu^{(s)}$.

<u>Lemma 5</u>

$$\begin{aligned}K_{s+1}(\cos\xi)=\;&\sum_{\nu=n+1}^{\infty}a_\nu I[T_\nu]\;-I[T_n]\sum_{\lambda=1}^{\infty}a_{(2\lambda+1)n}\\&-{\sum_{l=0}^{n-1}}^{*}\left(I[T_l]\sum_{\lambda=1}^{\infty}\Big(a_{2\lambda n+l}+a_{2\lambda n-l}\Big)\right)\,,\end{aligned}$$

where $\sum^*$ means that the first term should be halved.

Proof: By an application of Lemma 4 we get

$$\begin{aligned}Q_{n+1}^{\mathrm{CC}}\left[\frac{1}{s!}\Big(\cdot-\cos\xi\Big)_+^{s}\right]&=\sum_{\nu=0}^{\infty}a_\nu Q_{n+1}^{\mathrm{CC}}[T_\nu]\\&=\sum_{\nu=0}^{n}a_\nu Q_{n+1}^{\mathrm{CC}}[T_\nu]+\sum_{\lambda=1}^{\infty}\sum_{l=-n+1}^{n}a_{2\lambda n+l}Q_{n+1}^{\mathrm{CC}}\Big[T_{2\lambda n+l}\Big]\\&=\sum_{\nu=0}^{n}a_\nu I[T_\nu]+\sum_{\lambda=1}^{\infty}\sum_{l=-n+1}^{n}a_{2\lambda n+l}Q_{n+1}^{\mathrm{CC}}\Big[T_{|l|}\Big]\\&=\sum_{\nu=0}^{n}a_\nu I[T_\nu]+\sum_{\lambda=1}^{\infty}\left({\sum_{l=0}^{n-1}}^{*}\Big(a_{2\lambda n+l}+a_{2\lambda n-l}\Big)I[T_l]+a_{(2\lambda+1)n}I[T_n]\right)\\&=\sum_{\nu=0}^{n}a_\nu I[T_\nu]+{\sum_{l=0}^{n-1}}^{*}I[T_l]\sum_{\lambda=1}^{\infty}\Big(a_{2\lambda n+l}+a_{2\lambda n-l}\Big)+I[T_n]\sum_{\lambda=1}^{\infty}a_{(2\lambda+1)n}\,.\end{aligned}$$

The derangement of the series in the last step is justified only if

$$\sum_{\lambda=1}^{\infty}a_{(2\lambda+1)n}\qquad\text{and}\qquad\sum_{\lambda=1}^{\infty}\Big(a_{2\lambda n+l}+a_{2\lambda n-l}\Big)$$

are convergent series. This is trivial, if $s > 0$; in the case $s = 0$ we have

$$\sum_{\lambda=1}^{\infty} a_{(2\lambda+1)n} = \frac{2}{\pi n} \sum_{\lambda=1}^{\infty} \frac{\sin\big((2\lambda+1)n\xi\big)}{2\lambda+1},$$

which is a well-known convergent series, for the second series see the next lemma.

If we combine the last formula with

$$I\left[\frac{1}{s!}\big(\cdot - \cos\xi\big)_+^s\right] = \sum_{\nu=0}^{\infty} a_\nu I[T_\nu], \tag{12}$$

then we have Lemma 5. But (12) is surely correct, if $\sum_{\nu=0}^{\infty} a_\nu I[T_\nu]$ converges uniformly, that is for $s \geq 1$. If $s = 0$, then $\sum_{\nu=0}^{\infty} a_\nu I[T_\nu]$ has bounded partial sums, for it is the expansion of a function of bounded variation (Bary [1] p.137), and this is sufficient for an application of Lebesgue's dominated convergence theorem.

Lemma 6

$$\sum_{\lambda=1}^{\infty}\Big(a_{2\lambda n+l} + a_{2\lambda n-l}\Big) = -\frac{2}{\pi}\left(\frac{\pi}{n}\right)^{s+1} (\sin\xi)^s \cos(l\xi)\, B_s\left(\frac{n\xi}{\pi}\right) + O\Big((l+1)n^{-s-2}\Big).$$

Proof: We have from Lemma 3

$$\begin{aligned}
&a_{2\lambda n+l} + a_{2\lambda n-l}\\
&= \frac{2}{\pi}(\sin\xi)^s \left(\frac{\sin\big((2\lambda n+l)\xi - s\frac{\pi}{2}\big)}{(2\lambda n+l)^{s+1}} + \frac{\sin\big((2\lambda n-l)\xi - s\frac{\pi}{2}\big)}{(2\lambda n-l)^{s+1}}\right) + O\Big((\lambda n)^{-s-2}\Big)\\
&= \frac{2(\sin\xi)^s}{\pi(2\lambda n)^{s+1}}\bigg(\Big(1-(s+1)\frac{l}{2\lambda n} + O\Big(\frac{l^2}{\lambda^2n^2}\Big)\Big)\sin\Big((2\lambda n+l)\xi - s\frac{\pi}{2}\Big)\\
&\qquad + \Big(1+(s+1)\frac{l}{2\lambda n} + O\Big(\frac{l^2}{\lambda^2n^2}\Big)\Big)\sin\Big((2\lambda n-l)\xi - s\frac{\pi}{2}\Big)\bigg) + O\Big((\lambda n)^{-s-2}\Big)\\
&= \frac{2(\sin\xi)^s}{\pi(2\lambda n)^{s+1}}\Big(2\sin\Big(2\lambda n\xi - s\frac{\pi}{2}\Big)\cos l\xi - 2(s+1)\frac{l}{2\lambda n}\cos\Big(2\lambda n\xi - s\frac{\pi}{2}\Big)\sin l\xi\Big)\\
&\quad + O\Big(l^2(\lambda n)^{-s-3}\Big) + O\Big((\lambda n)^{-s-2}\Big).
\end{aligned}$$

If we use now (8), we obtain

$$\begin{aligned}
\sum_{\lambda=1}^{\infty}\Big(a_{2\lambda n+l} + a_{2\lambda n-l}\Big) &= -\frac{2}{\pi}\left(\frac{\pi}{n}\right)^{s+1}(\sin\xi)^s\cos(l\xi)\,B_{s+1}\left(\frac{n\xi}{\pi}\right)\\
&\quad -\frac{2}{\pi}\left(\frac{\pi}{n}\right)^{s+2}(\sin\xi)^s(s+1)l\sin(l\xi)\,B_{s+2}\left(\frac{n\xi}{\pi}\right)\\
&\quad + O\Big(l^2n^{-s-3}\Big) + O(n^{-s-2}),
\end{aligned} \tag{13}$$

and Lemma 6 follows.

<u>**Lemma 7**</u> Let f be a 2π-periodic continuous function of bounded variation. Denote by $\sum\limits_{\nu=0}^{\infty}\left(a_\nu \cos \nu x + b_\nu \sin \nu x\right)$ the FOURIER expansion of f. Then we have

$$\lim_{n\to\infty} \frac{1}{n} \sum_{\nu=1}^{n} \nu\sqrt{a_\nu^2 + b_\nu^2} = 0.$$

This is a theorem of N. WIENER. The proof can be found in BARY [1] p.212-215.

<u>**Lemma 8**</u>

$$\begin{aligned} &-\sum_{l=0}^{n-1}{}^{*} \left(I[T_l] \sum_{\lambda=1}^{\infty}\left(a_{2\lambda n+l} + a_{2\lambda n-l}\right)\right) \\ &\qquad = \left(\frac{\pi}{n}\right)^{s+1} (\sin\xi)^{s+1} B_{s+1}\left(\frac{n\xi}{\pi}\right) k(\cos\xi) \;+\; o(n^{-s-1}). \end{aligned} \tag{14}$$

Proof: From Lemma 6 we get

$$\begin{aligned} &-\sum_{l=0}^{n-1}{}^{*} \left(I[T_l] \sum_{\lambda=1}^{\infty}\left(a_{2\lambda n+l} + a_{2\lambda n-l}\right)\right) \\ &\qquad = \left(\frac{\pi}{n}\right)^{s+1} (\sin\xi)^{s} B_{s+1}\left(\frac{n\xi}{\pi}\right) \sum_{l=0}^{n-1}{}^{*} \frac{2}{\pi} I[T_l] \cos l\xi \\ &\qquad\quad + O(n^{-s-1}) O\left(\frac{1}{n}\sum_{l=0}^{n-1}{}^{*} (l+1)\left|I[T_l]\right|\right). \end{aligned} \tag{15}$$

Now the numbers

$$\begin{aligned} \frac{2}{\pi} I[T_l] &= \frac{2}{\pi}\int_{-1}^{1} T_l(x)k(x)\,dx = \frac{2}{\pi}\int_{0}^{\pi} \cos(lt)k(\cos t)\sin t\,dt \\ &= \frac{1}{\pi}\int_{-\pi}^{\pi} k(\cos t)\,|\sin t|\cos(lt)\,dt \end{aligned}$$

are FOURIER coefficients of the function $\hat{k}(\cos\cdot)$. Our assumptions on $\hat{k}$ guarantee the uniform convergence, that is

$$\sum_{l=0}^{n-1}{}^{*} \frac{2}{\pi} I[T_l] \cos(l\xi) = k(\cos\xi)\,|\sin\xi| \;+\; o(1).$$

Using this for the first term of (15) and Lemma 7 for the second term, we obtain Lemma 8.

<u>**Lemma 9**</u>

$$\sum_{\nu=n+1}^{\infty} a_\nu I[T_\nu] = o(n^{-s-1}). \tag{16}$$

Proof: Lemma 3 implies that it is sufficient to prove

$$\sum_{\nu=n+1}^{\infty} \nu^{-s-1}\Big|I[T_\nu]\Big| = o(n^{-s-1}). \tag{17}$$

Partial summation leads to

$$\begin{aligned}\sum_{\nu=n+1}^{m} \nu^{-s-1}\Big|I[T_\nu]\Big| &= \sum_{\nu=n+1}^{m} \nu^{-s-2}\Big(\nu\Big|I[T_\nu]\Big|\Big)\\ &= -n^{-s-2}\sum_{\nu=1}^{n}\nu\Big|I[T_\nu]\Big| + \sum_{\kappa=n}^{m-1}\Big(\Big(\kappa^{-s-2}-(\kappa+1)^{-s-2}\Big)\sum_{\nu=1}^{\kappa}\nu\Big|I[T_\nu]\Big|\Big)\\ &\quad + m^{-s-2}\sum_{\nu=1}^{m}\nu\Big|I[T_\nu]\Big|.\end{aligned}$$

According to Lemma 7 we have $\frac{1}{m}\sum\limits_{\nu=1}^{m}\nu\Big|I[T_\nu]\Big| \to 0$, hence we get in the limit $(m\to\infty)$

$$\sum_{\nu=n+1}^{\infty} \nu^{-s-1}\Big|I[T_\nu]\Big| = -n^{-s-2}\sum_{\nu=1}^{n}\nu\Big|I[T_\nu]\Big| + \sum_{\kappa=n}^{\infty}\kappa\Big(\kappa^{-s-2}-(\kappa+1)^{-s-2}\Big)\Big(\frac{1}{\kappa}\sum_{\nu=1}^{\kappa}\nu\Big|I[T_\nu]\Big|\Big),$$

and thus by Lemma 7 we obtain (17).

Now the proof of the theorem is quite simple. We have to introduce (14) and (16) in Lemma 5 and to observe

$$\begin{aligned}I[T_n]\sum_{\lambda=1}^{\infty} a_{(2\lambda+1)n} &= O\left(I[T_n]\sum_{\lambda=1}^{\infty}(2\lambda+1)^{-s-1}n^{-s-1}\right) = n^{-s-1}O\Big(I[T_n]\Big)\\ &= o(n^{-s-1}).\end{aligned}$$

Finally, in the special case $k=1$ we have

$$I[T_l] = \begin{cases} 0 & l \text{ odd} \\ -2(l^2-1)^{-1} & l \text{ even.}\end{cases}$$

The modifications in the preceding proof, which are necessary to get the more precise error estimation in this special case, are obvious, apart from one point. In the proof of Lemma 8 we have to replace Lemma 6 by the more precise result (13), and we have to observe that

$$\sum_{l=0}^{n-1}{}^{*}\, I[T_l]\,l\sin(l\xi) = -2\sum_{l=1}^{m}\frac{2l}{4l^2-1}\sin(2l\xi) = -2\cos\xi\sum_{l=0}^{m-1}\frac{\sin\Big((2l+1)\xi\Big)}{2l+1} - \frac{\sin(2m\xi)}{2m+1}$$

(where $m := \left\lfloor\frac{n-1}{2}\right\rfloor$) is bounded with respect to n and ξ.

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